SIMULATION OF FIRES WITH RADIATIVE HEAT TRANSFER

by

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INTRODUCTION

Thermal radiation is the dominant mode of heat transfer in very large fires. Even in small pool fires (diameter of 0.1–0.3 m) radiative feedback to the fuel surface is significant [1]. The purpose of this paper is to describe a model of radiative transport in gases that is suitable for use with a large eddy simulation (LES) approach for fire dynamics developed at NIST [2, 3]. This LES model of convective transport and combustion heat released was developed by distinguishing between physical processes that can be explicitly computed and those that operate at length and time scales too small to be resolved (i.e., subgrid). The same strategy will be attempted here for the thermal radiation generated by the fire. The starting point is the radiative transport equation for gases. For the present purposes it is sufficient to understand that the fluid mechanics is calculated on an Eulerian finite difference grid in rectangular coordinates. The velocity and temperature fields so calculated are assumed to be large scale phenomena resolvable on the grid. The combustion phenomena that drive the flow are assumed to be of subgrid scale, whose consequences can be represented by Lagrangian "thermal elements". These elements release sensible energy into the gas as they are convected with the large scale fluid motion. A description and justification of this procedure can be found in [3] and [4].

In the analysis of radiative transport, it will be assumed that part of the energy released as a result of the combustion processes is emitted as thermal radiation. This implies that the emission processes are also subgrid scale, and cannot be calculated on a macroscopic grid equivalent to that used for the fluid mechanics. The absorption and transport of radiation however, are both assumed to take place on scales set by the large scale fluid motion and the enclosure or scenario geometry, if any. Thus, these phenomena are resolved explicitly in the model and computations described below. This implies that the radiation fields are far from equilibrium in the fire scenarios of interest here. In effect, the radiation is treated in a manner analogous to the combustion phenomena that generate it. The crucial point in the analysis is that the *energy release* and not the temperatures in the subgrid scale phenomena that must be captured. The subgrid combustion physics also controls the soot generation. This is accounted for by defining the local soot mass distribution as a property associated with the "thermal elements". This information can be converted into grid-based information as needed, in exactly the same way as the combustion heat release is for the computation of the convective transport.

THE RADIATIVE TRANSPORT MODEL

The starting point for the analysis is the radiative transport equation for a non-scattering grey gas [5].

$$\Omega \cdot \nabla I(\mathbf{r}, \Omega) = \kappa(\mathbf{r}) \left(\frac{\sigma T(\mathbf{r})^4}{\pi} - I(\mathbf{r}, \Omega) \right). \tag{1}$$

Here, $I(\mathbf{r}, \Omega)$ is the radiant intensity, defined so that $I(\mathbf{r}, \Omega)\mathrm{d}\Omega$ is the radiant energy at a point $\mathbf{r}$ passing through a unit area per unit time through the element of solid angle $\mathrm{d}\Omega$ centered about the direction Ω. The grey gas absorption coefficient is $\kappa(\mathbf{r})$, and the local temperature is $T(\mathbf{r})$. The quantity σ is the Stefan-Boltzmann constant. Both the spectral dependence of the radiation and the scattering have been ignored because in the emitting regions where they are likely to be important, the relevant processes cannot be spatially resolved; while in the spatially extended soot clouds, absorption is the most important mechanism.

The radiant heat flux vector $\mathbf{q}(\mathbf{r})$ can be defined in terms of the radiant intensity as follows:

$$\mathbf{q}(\mathbf{r}) = \int \Omega I(\mathbf{r}, \Omega)\mathrm{d}\Omega. \tag{2}$$

Here, the integral is taken over all 4π steradians since the radiation at a point can be coming from any direction. Similarly, the integrated radiant intensity $U(\mathbf{r})$ is defined as:

$$U(\mathbf{r}) = \int I(\mathbf{r}, \Omega)\mathrm{d}\Omega. \tag{3}$$

Note that $U(\mathbf{r})/c$ is the radiant energy density; c is the speed of light. Using this definition and integrating equation (1) over all Ω yields the conservation of radiant energy equation

$$\nabla \cdot \mathbf{q}(\mathbf{r}) = \kappa(\mathbf{r}) \left[4\sigma T(\mathbf{r})^4 - U(\mathbf{r})\right]. \tag{4}$$

This equation is simply a statement that the net radiant energy flux out of any region occupied by the gas is the difference between that emitted and absorbed in the volume under consideration. This energy exchange between the radiation field and the gas is what couples the convective transport and radiative transport in the bulk of the gas. The coupling at gas/surface interfaces will be considered briefly below.

The dependence of each physical quantity on $\mathbf{r}$ and Ω is shown explicitly since this constitutes the principal mathematical and computational difficulty associated with radiative transport. Since the radiant intensity at each instant of time depends on five independent variables (Ω is a unit vector), the direct solution of equation (1) is prohibitively difficult. Some drastic approximation is needed; especially when the high resolution grids needed for convective transport are considered. There are two basic choices available. First, the spatial resolution can be reduced to the point where the number of grid points in each direction is comparable to the number of direction cosines retained for computational purposes. Alternatively, the high spatial resolution could be retained but an explicit simplifying form can be chosen for the dependence of the radiant intensity on Ω. The latter choice is made here.

There are two main reasons for this choice. First, since high spatial resolution is needed for the description of convective transport, it follows that the sources and sinks of radiation that appear in the radiant energy equation (4) must have considerable fine structure. Cutting back on the spatial resolution to accommodate a high angular resolution might well undermine the description of convective transport. Second, the "diffusion approximation" in the sense of [5] gives results that are accurate enough for the present application, especially when the approximations already made in the radiative transport equation (1) are taken into account.

To proceed, following [5] note that equation (4) gives one relationship between U and $\mathbf{q}$. It arises from the zeroth moment of equation (1) with respect to Ω. If a suitable functional form for I as a function of Ω that preserves the next (vector) moment of this equation can be found

involving only U and $\mathbf{q}$, then a closed system of equations will result. The existence of such a form is well known; in the present notation it can be written as:

$$I(\mathbf{r},\ \Omega) = \frac{1}{4\pi}\left(U(\mathbf{r}) + 3\mathbf{q}\cdot\Omega\right). \tag{5}$$

This choice preserves the first four scalar moments of the radiative transport equation, and closes the system with the relation

$$\nabla U(\mathbf{r}) = -3\ \kappa(\mathbf{r})\ \mathbf{q}\ (\mathbf{r}). \tag{6}$$

With this relation for the radiant heat flux vector and equation 4 the conservation equation for the integrated intensity is

$$\nabla\cdot\frac{1}{\kappa(\mathbf{r})}\nabla U(\mathbf{r}) - 3\kappa(\mathbf{r})U(\mathbf{r}) = -3\kappa(\mathbf{r})4\sigma T^4(\mathbf{r}). \tag{7}$$

Equation 7 is known as the P1 approximation to the radiation transfer equation [6].

SEMI-INFINITE DOMAIN SOLUTION

A formal solution to the radiative transport problem in a semi-infinite domain can be developed based on concepts introduced by Baum and Mell [7]. The gas occupies the half space $y \geq 0$. It consists of a background of weakly absorbing gas with $\kappa = \kappa_\infty$ interspersed with a number of compact regions emitting with a total radiative power $\tilde{Q}_n$. The centroid of each region is located at $\mathbf{r} = \mathbf{r}_n$. The boundary is at temperature $T = T_w(x, 0, z)$. There are two objectives of the analysis. First, it shows how a model based on a large number of subgrid scale interacting emitters embedded in an absorbing background can be used to represent the radiation from an isolated fire plume. Then, the same result is obtained numerically to demonstrate that the use of efficient elliptic partial differential equation solvers combined with the notion of a boundary as a strongly absorbing extension of the computational domain allows highly resolved radiation fields to be obtained at relatively modest computational cost.

Far from any of the regions of elevated temperature, $U \to U_\infty$, where $U_\infty = 4\sigma T_\infty^4$. Thus, for this problem the model equations can be written as:

$$U = U_\infty + V(\mathbf{r}), \tag{8}$$

$$\nabla^2 V - 3\kappa^2 V = -3\kappa^2 4\sigma\left(T^4 - T_\infty^4\right). \tag{9}$$

The only boundary condition is that $V \to 0$ at infinity.

We now make explicit use of the fact that the length scale $(\kappa_\infty)^{-1}$ is assumed to be much larger than any of the sphere radii R_n. Viewed on the large scale, the emitters in the gas phase are a collection of point sources of unknown strength $\tilde{Q}_n$. Thus, the solution on the $(\kappa_\infty)^{-1}$ scale satisfies the equation:

$$\nabla^2 V - 3\kappa_\infty^2 V = -3\kappa_\infty \sum_{n=1}^{N} \tilde{Q}_n \delta\left(\mathbf{r} - \mathbf{r}_n\right). \tag{10}$$

The solution for V must vanish far from the boundary, while at $y = 0$ [7]:

$$V - \frac{1}{\sqrt{3\kappa_\infty}}\frac{\partial V}{\partial y} = 4\sigma\left(T_w^4 - T_\infty^4\right). \tag{11}$$

The solution can be expressed in terms of a Green's function $G(\mathbf{r}, \mathbf{r}_0)$ that physically represents the solution corresponding to a point source in the presence of a cold boundary at temperature T_∞ [7]:

$$V(\mathbf{r}) = -3\kappa_\infty \sum_{n=1}^{N} \tilde{Q}_n G(\mathbf{r}, \mathbf{r}_n) + V_s(\mathbf{r}), \tag{12}$$

$$V_s(\mathbf{r}) = -\sqrt{3}\kappa_\infty \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r}, \mathbf{r}_s) 4\sigma \left(T_w^4 - T_\infty^4\right) \mathrm{d}x_s \, \mathrm{d}z_s \tag{13}$$

The Green's function is

$$G = G_\infty(\mathbf{r} - \mathbf{r}_0) + G_\infty(\mathbf{r} - \mathbf{r}_1) + K. \tag{14}$$

Here G_∞ is the fundamental Green's function associated with the P1 equation

$$G_\infty(\mathbf{r} - \mathbf{r}_0) = -\frac{1}{4\pi \mid \mathbf{r} - \mathbf{r}_0 \mid} \exp\left(-\sqrt{3}\kappa \mid \mathbf{r} - \mathbf{r}_0 \mid\right). \tag{15}$$

and K is

$$K = \frac{\sqrt{3}\kappa_\infty}{2\pi} \exp\left(\sqrt{3}Y\right) E_1\left[\sqrt{3}\left(Y + \sqrt{Y^2 + \lambda^2}\right)\right] \tag{16}$$

with $\lambda = \kappa_\infty \sqrt{\left((x - x_0)^2 + (z - z_0)^2\right)}$ and $Y = \kappa_\infty (y + y_0)$ [7].

The Green's function is axially symmetric, depending on the three variables λ, $\kappa_\infty y$, and $\kappa_\infty y_0$.

The solution to this radiative transport problem can be regarded as complete once the boundary temperature T_w and the strength of the emitters $\tilde{Q}_n$ are known. The wall temperature is determined in practice by an energy balance in the solid which takes into account heat conduction. The source strength must either be calculated from a local analysis on the scale of the emitting material or specified as a fraction of the chemical heat release which drives the fire. Since the small scale phenomena which control the chemical heat release are subgrid scale in the fire simulations for which this model is intended, the details of the local model are not important in the present context. However, it is *very* important to distinguish between radiant energy liberated locally as a result of combustion, and the net energy escaping to remote portions of the spatial domain of interest. The former quantity may be regarded as "input" into the radiative transport problem, while the latter must be part of the solution.

SIMULATION OF AN ISOLATED FIRE PLUME

A typical distribution of thermal elements in a large eddy simulation (LES) of a square pool fire is shown in Figure 1; L_x, L_z and L_y are the physical dimensions of the domain in the two horizontal and vertical directions, respectively, The dark colored points correspond to thermal elements that locate active combustion and the lighter colored points are where combustion the thermal elements have burned out. On the base of the domain the radiative flux on the solid surface is shown by greyscale contours (lighter shading corresponds to a larger flux). Details regarding the formulation of the LES model are given in Baum *et al.* [2, 4]. To date the LES calculations have assumed that a fixed fraction of the chemical heat release is lost by radiation to surroundings which are radiatively nonparticipating. Time averaged LES results and experimental correlations for an isolated fire plume are in good agreement [2]. Indeed, for

problems of practical interest a thermal radiation model is the most important improvement to the large eddy simulation's description of large scale thermal transport. To this end, the analytical results of the previous section [i.e., equation (12)] were used to test the accuracy of the numerical solution of the P1 approximation for the case of an isolated fire plume with a constant absorption coefficient in the gas. The solid boundary temperature was assumed to be ambient and the distribution and strengths of the point source emitters were obtained from LES results such as those shown in Figure 1.

Within the context of the large eddy simulation the net volumetric rate of chemical heat release, which appears in the energy equation, is

$$\dot{q}_c(\mathbf{r},t) = \sum_n \dot{Q}_c(t - t_{i,n})\delta(\mathbf{r} - \mathbf{r}_n(t)). \tag{17}$$

Here $\dot{Q}_c$ is the prescribed net volumetric chemical heat release rate of a thermal element; $\mathbf{r}_n(t)$ is the position of thermal element n and $t_{i,n}$ is the time at which thermal element n leaves the fuel bed. The value of $\dot{Q}_c$ and its time history are defined such that the fire's total heat release rate and the average flame height are consistent with experimental results. The LES conservation equations for the radiant energy and the integrated intensity are

$$\nabla \cdot \mathbf{q}(\mathbf{r},t) = \sum_n \dot{Q}_r(t;n)\delta(\mathbf{r} - \mathbf{r}_n(t)) - \kappa(\mathbf{r})V(\mathbf{r}), \tag{18}$$

and

$$\nabla \cdot \frac{1}{\kappa(\mathbf{r})}\nabla V(\mathbf{r}) - 3\kappa(\mathbf{r})V(\mathbf{r}) = -3\sum_n \dot{Q}_r(t;n)\delta(\mathbf{r} - \mathbf{r}_n(t)). \tag{19}$$

Here the net volumetric rate of radiant emission for element n is

$$\dot{Q}_r(t;n) = \beta\dot{Q}_c(t;n)\delta(\mathbf{x} - \mathbf{x}_n). \tag{20}$$

Where β is the prescribed fraction of the chemical heat release rate that is radiatively emitted.

Given the spatial distribution of $\dot{Q}_c$ from the LES calculation, equation (19) was solved with an absorption coefficient which follows a step function in the vertical direction

$$\kappa(\mathbf{r}) = \begin{cases} \kappa_\infty & : \quad y > 0 \\ \kappa_w & : \quad y \le 0 \end{cases} \tag{21}$$

A control volume numerical solution approach to equation (19) was used with Fast Fourier transforms in the horizontal directions and Gauss elimination in the vertical direction (direction of variable absorption). The staggered grid used in the LES hydrodynamic calculation was also used in the gas phase part of the radiation calculation. Additional grid points were added to account for absorption in the solid phase. Retaining continuity of both the integrated intensity and the radiative flux across the gas/solid absorption interface was handled in a manner analogous to methods for thermal conductivity interfaces [8].

Figures 2 and 3 show results from a LES simulation of a methanol pool fire. The pool is 30 cm square; the calculational domain was comprised of 64 × 64 × 128 cell volumes representing a physical domain of $L_x = L_z$ =1.28 m on the sides and L_y = 2.56 m tall. The gas and solid phase absorptions, κ_∞ and κ_w, were defined such that $L_x\kappa_\infty = L_z\kappa_\infty = 4$ and $L_w\kappa_w = 1.25$ (where L_w is the thickness of the solid phase in the radiation calculation). The radiative heat loss fraction was $\beta = 0.2$. Based on experimentally measured mass burning rates the prescribed

heat release rate of the pool fire was 23 kW. The active combustion or flame zone was represented by approximately 36,000 of a total of roughly 80,000 thermal elements.

The numerical calculations were performed on an IBM/RISC 6000 workstation. The computational cost of the large eddy simulation was 20×10^{-6} *cpu s/(cell · timestep)*; approximately 8 h of CPU time was required for 10 s of simulated real time. Obtaining the integrated intensity from the P1 approximation required 1.3×10^{-6} and 5×10^{-2} *cpu s/(cell · timestep)* with the FFT based method and the analytical solution (which used NAG routines to evaluate the exponential integral), respectively. From these timings it is clear that on the scale of the overall LES calculation the P1 approximation is very efficient computationally. Including the P1 approximation in the LES calculation did not require a reduction in the spatial resolution used for the hydrodynamics. Note that this would not have been the case for more expensive models with angular dependence such as the discrete ordinates method.

Figure 2 shows a vertical profile of the integrated intensity above the center of the pool from both the analytical and numerical solutions of equation (10). The gas/solid interface is at $y = 0$; negative values of the horizontal axis correspond to locations within the solid. The numerical solution of equation 19 is in excellent agreement with the analytical solution (solid line) of equation 12. This agreement allows one to calculate the radiation flux on the surface from the value of the integrated intensity by using equation (11). The radiation flux on the surface is show in Figure 3. Note that the absorption coefficient of the pool and its surroundings are identical. Again the numerical result is in excellent agreement with the analytical values (solid lines). The FFT based method is clearly an accurate and computationally efficient method for including the P1 approximation in large eddy simulations of isolated fire plumes with a constant absorption coefficient.

It is of interest to determine how well plume correlations [9] work in cases where radiative absorption is significant. Results from large eddy simulations of a 60 kW, 30 cm square pool fire with and without the P1 approximation are shown in Figure 4. The domain size was $L_x = L_z = 1.5$ m and L_z=3.5 m; LES results were time averaged over 15 s. For the simulations with a radiation model the absorption coefficient was defined in two ways: as in equation (21) and according to

$$\kappa_g = \begin{cases} \kappa_{ot} & : \quad 0 < y \leq y_{sp} \\ \kappa_{ot} + \frac{\kappa_\infty - \kappa_{ot}}{y_{max} - y_{sp}}(y - y_{sp}) & : \quad y \geq y_{sp} \end{cases} \tag{22}$$

where y_{sp} was an assumed smoke point height; $y_{max} = L_z$; and κ_{ot} was a value of the absorption coefficient which was small enough to ensure that the gas was radiatively nonparticipating below the smoke point height. The results of Figure 4 were based on $y_{sp} = 20$ cm, $\kappa_{ot} = 10^{-6}\text{m}^{-1}$ and $\beta = 0.35$. The absorption coefficient was defined according to equation (22) in order to mimic to some degree real fires in the sense that little absorption due to soot occurs below a height called the smoke point. Results in Figure 4 from simulations without a radiation model were obtained in two ways, first by assuming that $\beta = 0.35$ with nonparticipating gas (this was a lower bound on the temperatures obtained from LES cases with a radiation model). The second way was with $\beta = 0$ so that all the chemical heat release was diffused into the gas (this put an upper bound on the temperatures, in locations where emission is present, from LES cases with a radiation model). In Figure 4(a) $\kappa_{ot} = \kappa_\infty = 10^{-6}\text{m}^{-1}$ the gas is radiatively nonparticipating for all cases; the $\beta = 0$ results have the highest temperature and the other three cases are in agreement with each other as expected. From the correlations, the continuous flame zone (in which emission is dominant) exists up to a height of 30 cm. In Figures 4(b,c,d) κ_∞ is successively increased by an order of magnitude. As κ_∞ increases LES results with radiation first deviate from each other and then nearly collapse again to the same curve (at very high ab-

sorption). Also, as κ_{∞} increases, temperatures from LES (with radiation) become significantly higher than those from the correlations in a 1 m range above the continuous flame zone.

The simple approach taken here for the spatial dependence of the absorption coefficient is an appropriate first step for including radiation transfer in an isolated plume. However, simulations with a more physically based fully three-dimensional absorption coefficient are required before more conclusive results can be obtained.

SUMMARY AND CONCLUSIONS

The grey gas P1 approximation to the radiative transport equation has been shown to be a suitable radiation model for use in large eddy fire simulations of the kind developed at NIST. This LES technique is based on the assumption that the chemical heat release and radiative emission occur on subgrid scales. With present day computers three-dimensional LES simulations of fire dynamics in which radiative heat transfer is not modeled are possible over scale ranges up to approximately two orders of magnitude. By averaging over the angular dependence the P1 approximation is a computationally efficient radiation model. Thus, using the P1 approximation in the LES approach did not compromise spatial resolution.

For the case of an isolated fire plume with a constant absorption coefficient a fast Fourier transform based numerical solution and the exact solution to the P1 approximation were compared. The numerical solution was found to be accurate and highly efficient computationally, requiring only a fraction of the LES computational cost. Time averaged LES centerline temperatures were compared to empirically based correlations. Agreement between the simulations and correlations degraded as the absorption coefficient increased.

Future developments of this approach will include the use of a three-dimensional multigrid numerical procedure for solving the P1 approximation equation. This will allow simulations of enclosed domains with obstacles and fully three-dimensional variable absorption in the gas phase (e.g., soot).

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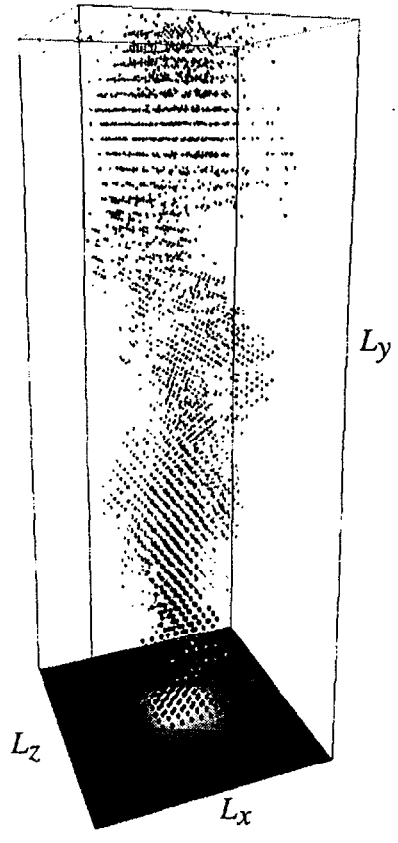


Figure 1: Thermal elements from a large eddy simulation of a square pool fire. L_x and L_z denote the two horizontal dimensions and L_y the vertical. Thermal elements which are dark correspond to locations of active combustion, lighter shading denotes elements that have burned out. The radiative flux on the bottom surface is shown by greyscale contours, lighter shading corresponds to a larger flux.

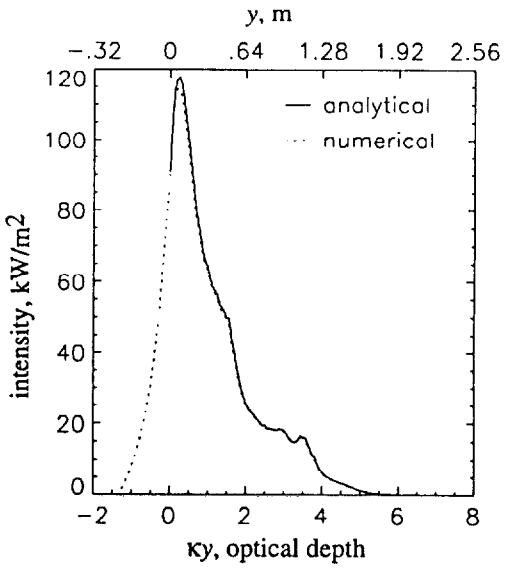


Figure 2: Vertical profile of the integrated intensity, V, above the center of the pool fire (23 kW, 30 cm square). Negative depth values correspond to points with the solid. The intensity from both the numerical (dotted line) and the analytical (solid line) solutions to the radiation transfer equation are shown.

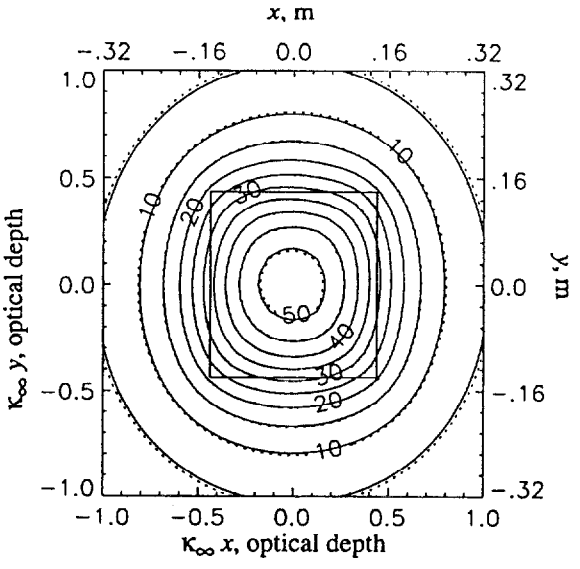
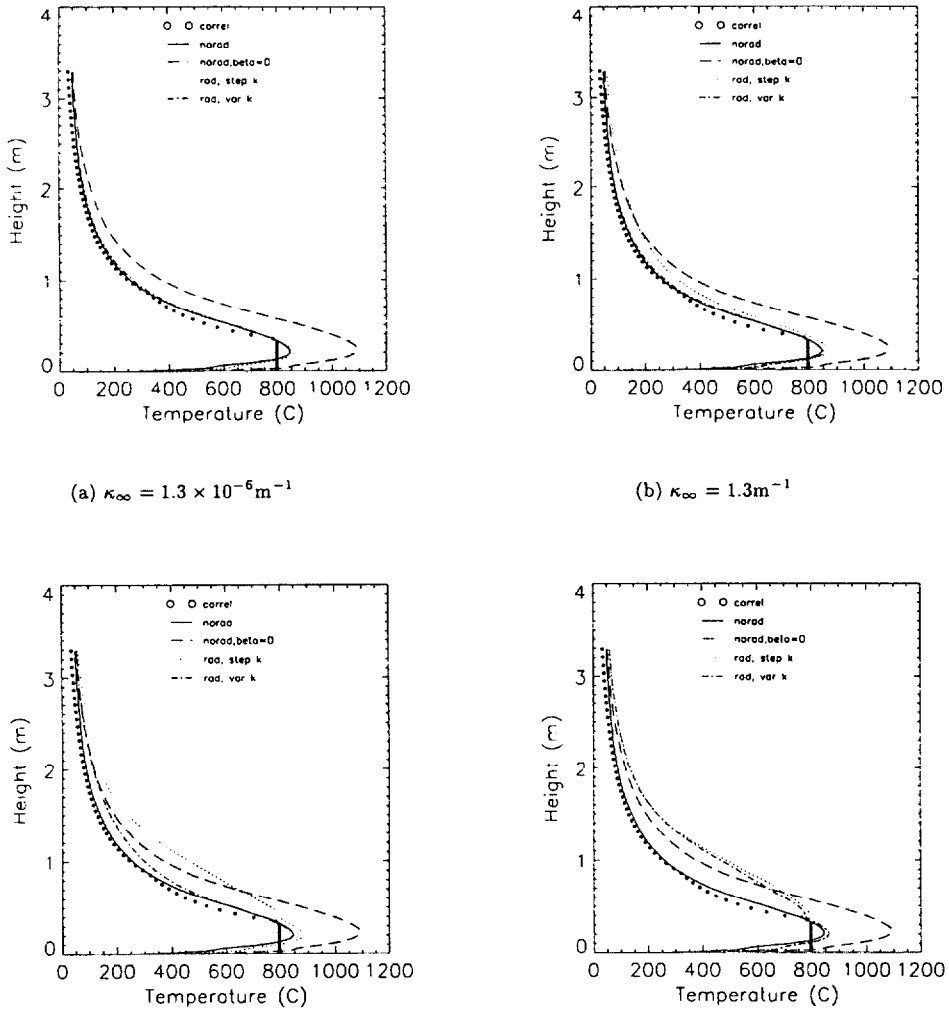


Figure 3: Radiation flux (kW/m^2) on the bottom surface. The square outline of the pool fire (23 kW, 30 cm square) is also shown. Solid lines correspond to the analytical solution and dotted to the numerical.



(a) $\kappa_\infty = 1.3 \times 10^{-6}\mathrm{m}^{-1}$

(b) $\kappa_\infty = 1.3\mathrm{m}^{-1}$

(c) $\kappa_\infty = 13.3\mathrm{m}^{-1}$

(d) $\kappa_\infty = 133\mathrm{m}^{-1}$

Figure 4: Comparison of time averaged large eddy simulation temperatures to empirically based plume correlations for four different gas absorption environments $\kappa_\infty = (1.3 \times 10^{-6}, 1.3, 13.3, 133)$ m^{-1}. The solid and dashed lines correspond to LES results without a radiation model: solid line case has $\beta = 0.35$, dashed line has $\beta = 0$ (i.e., no fraction of the chemical heat release is radiatively emitted). The dotted and dash/dot lines correspond to LES results with a radiation model: dotted case has a constant absorption coefficient $\kappa_g = \kappa_\infty$ in the gas, dash/dot has a variable κ_g in the gas [equation (22)].